Computational Chemistry in Combustion

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Abstract

The mechanistic steps in the combustion or gasification of coal are not well understood due to the large and complex nature. We are using computational chemistry to understand the important aspects of reactivity for large polycyclic aromatic hydrocarbons (PAHs) and their mechanisms of oxidation. The energy required to cleave C-H and N-H bonds in representative aromatic rings have been determined. We have also explored the decomposition pathways for arylperoxy radicals derived from the monocyclic rings. The modes of attack for radicals of importance to combustion (H, O, and OH) have been examined for their reactivity with monocyclic analogs of PAHs.